Organization: University of California, Berkeley

Title: Simulation of Biomolecular Nanomechanical Systems (BioNEMS)

MTO Simbiosys

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Project Goals

To develop multiscale modeling and simulation tools, which can be employed to establish design rules that can assist the development of biomolecular microsystems.

Technical Approach

Self-consistent-field calculations, Monte-Carlo simulations, CFD-ACE 3-dimensional fluid dynamic simulations, and experiments using a microfluidic chip are used synergistically to study deflection of cantilevers due to surface biomolecular interactions.

Recent Accomplishments

- Completed self-consistent-field calculations and Monte-Carlo simulations of single and double stranded DNA molecules adsorbed on cantilevers; quantified the deflection resulting from hybridization reactions.
- Developed a cantilever microarray chip along with approaches for functionalizing individual cantilever pixels and simultaneously measuring deflections of multiple cantilever beams with resolution of ≈ 1 nm.
- Developed 3D computational model of reaction chamber with microcantilever thereby assisting the design of microfluidic components.
- Performed microfluidic flow and DNA hybridization calculations on stiff cantilevers

Six-Month Milestones

- Complete the development of theoretical framework for predicting cantilever deflections at equilibrium for both single stranded and double stranded DNA, given the grafting density.
- Develop experimental method for determining grafting density.
  - Use multiplexed experimental method for measuring deflections as a function of various parameters with close synergy with theory.
  - Complete (a) design of microfluidic platform (stop chambers, interconnects etc. for multiplexing) (b) analysis of cantilever structural mechanics
- Coupled flow-induced deflection & DNA hybridization simulations

Team Member Organizations

Vinod Makhijani, CFDRC.

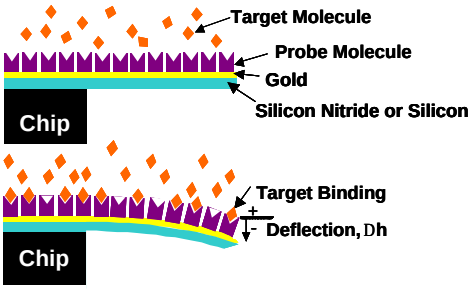


Fig. 1

The platform for our studies is a microcantilever beam whose one surface will be functionalized with probe biomolecules **(Fig. 1).**

We have used self-consistent-field calculations and Monte-Carlo simulations to calculate cantilever deflection upon hybridization of single stranded probe DNA molecules. **Fig. 2** shows the dependence of cantilever deflection on the number of nucleotides that make up the DNA molecules. These results are in good agreement with experiments.

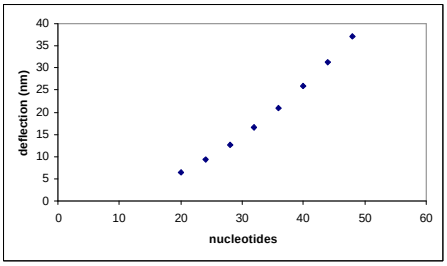


Fig. 2

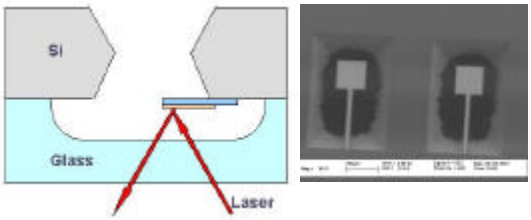
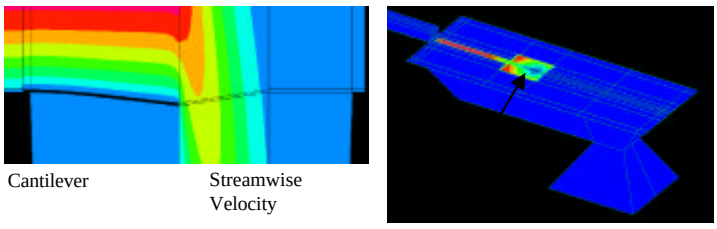


Fig. 3

Fig. 3 (left) shows a cross section of the chip where the cantilever is fabricated a silicon wafer and an etched glass wafer is bonded to it to create microwells for each cantilever pixel. **Fig. 3 (right)** shows an electron micrograph of the top view of part of the cantilever microarray.

Examples of simulations using this code developed at CFDRC that have proven useful in chip design are shown in **Fig. 4.**



Cantilever Streamwise Velocity

Fig. 4